Topic of Research: Study of Hydrogenic Impurity States in Quantum wires and Quantum Dots

Proposed Synopsis for Ph.D. Registration

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1. State of Art

Low-dimensional nanostructures have unique features. Some of the low dimensional structures are quantum wells, quantum dots, nanowires, and 2D materials. They usually need understanding of advanced condensed matter physics and nanotechnology. The distinct properties of these low dimensional structures are due to confined electrons in reduced spatial dimensions [1-3]. We can define such type of materials by Quantum confinement effects. In such type of devices movement of electron is limited in one or more directions. This causes discrete energy levels and change in electronic characteristics. This special behavior of such type of nanostructures is useful for many applications. They are favorable in semiconductor technology, optoelectronics, and quantum computing [4-6].

1.1 Role of Impurities in Low-Dimensional Systems:

Impurities play very important role in physical and electronic properties of such type of materials. Impurities can be added intentionally or unintentionally. In bulk materials, new energy levels are created within the bandgap due to impurities which affects conductivity and charge transport. In case of low-dimensional nanostructures, impurities have a stronger effect because of the confined electrons in reduced spatial dimensions. That's why in low dimensional nanostructures their properties are influenced more significantly by the added impurities [7,8].

As these impurities creates localized states in low dimensional system therefore, they change energy spectrum which effects some other properties like carrier mobility, optical absorption, and magnetic ordering [9,10]. Different types of phenomena can be induced due to these impurities which are as follows:

1.1.1 Quantum Confinement Effects:

A sharp change in density of states is observed when impurities interact with confined electrons. This modifies electronic transitions.

1.1.2 Optical Transitions and Luminescence:

Impurities can change the optical properties of quantum wells and quantum dots. They often cause enhanced or reduced luminescence. This is important for lasers and light-emitting diodes (LEDs).

1.1.3 Carrier Localization:

Impurity states can trap charge carriers. This reduces their mobility and changes the material conductivity. It is significant for devices like transistors and sensors.

1.2 Types of Impurities

Hydrogen impurities affect low-dimensional materials like 2D materials, 1D systems, and quantum dots. They can change electronic, optical, and chemical properties. These impurities can act as hydrogen donors or acceptors. This depends on their interaction with the material lattice and electronic structure [1]. Below is an explanation of hydrogen donor and hydrogen acceptor impurities. It includes examples in various low-dimensional systems:-

1.2.1 Hydrogen Donor Impurities:

Hydrogen donor impurities donate electrons (negative charge carriers) to the system. This happens when hydrogen atoms bond with a lattice site. This creates a negative charge center and makes the system more n-type (electron-rich) [11]. Some examples of this type of impurity are as follows:-

- **Graphene**: Hydrogenated graphene (graphene) can exhibit donor behavior when hydrogen atoms are attached to carbon atoms in a way that facilitates electron donation into the conduction band. This can lead to enhanced n-type behavior in graphene-based materials.
- **2D Semiconductors:** In 2D materials like MoS_2, hydrogen atoms (from hydrogenated compounds or adsorbed species) can act as donor impurities,

increasing the electron concentration in the material and changing its electronic properties.

- **Silicon Nanostructures**: Hydrogen passivation in silicon nanowires or quantum dots can result in donor-like states, altering the electron density and modifying the band gap.

1.2.2 Hydrogen Acceptor Impurities

Hydrogen acceptor impurities accept electrons from the material. This creates positive charge carriers (holes) in the system. It happens when hydrogen pulls electrons away from the lattice. This makes the material more p-type (hole-rich) [11]. Some examples [12] of this type of impurity are as follows:-

- **Graphene:** Hydrogen atoms attach to carbon atoms in hydrogenated graphene. This can make hydrogen act as an acceptor impurity. It pulls electron density away from the carbon lattice, leading to p-type doping. This depends on hydrogen coverage and defect configurations.
- **Transition Metal Dichalcogenides (TMDs):** In materials like MoS_2 or WS_2, hydrogen can adsorb on the surface or interact with defects. This creates acceptor states, reducing electron density and causing p-type behavior.
- **Silicon and Gallium Arsenide:** In semiconducting nanostructures like silicon, hydrogen can act as an acceptor impurity. When hydrogen is adsorbed on the surface or in the lattice, it creates hole carriers and promotes p-type conduction.

1.3 Importance of Studying Impurity States:

It is very important to understand impurities and their effects in low dimensional system for further research. If doping has done in controlled and appropriate way it changes electronic properties for specific device and enhance their performance like n-type or p-type regions in transistors. On the other hand unintentional impurities can harm the device performance by introducing unwanted energy states, reducing carrier lifetime or mobility.

Impurities play role of quantum bits (qubits) in quantum technologies, therefore to study material properties at nanoscale it is very important to develop understanding of impurity states.

1.4 Challenges and Opportunities:

The main challenge in this field of low dimensional nanostructure is to control impurity states. As impurities which interacts with host material can cause more complex effects therefore an appropriate model and computational techniques are required for its understanding. If materials are designed with specific impurities they leads to new applications like nanotechnology-based sensors, photonics etc.

The study of impurity states in low-dimensional nanostructures has a wide range of practical application. The study of interaction of impurities with such type of systems leads to design better electronics and nano technology devices.

2. Problem to be investigated

The following aspects will be mainly investigated in our proposed research work:

2.1 Study impurity states in quantum dots of various geometries. This includes rectangular, spherical, and cylindrical geometries. Emphasis will be given on the study of quantum dots with cylindrical geometry and its limiting behavior.

2.2 To investigate the impurity states in quantum wires of polygonal cross-section and of cylindrical cross-section. The cross-sectional plane may include simply-connected or multiply-connected domains.

2.3 The theoretical results will be computed numerically and will be compared with experimentally available data as far as possible.

3. Objectives of the investigation and motivation

The main goal of this study is to explore how impurity states affect the electronic properties of nanostructures. These include quantum dots and quantum wires. These nano systems have confined electron motion and show novel phenomena. They are very sensitive to impurities, making them ideal for theoretical exploration.

The nanostructures like quantum dots and quantum wires with controlled impurity states have vast application in quantum computing and other nanoscale devices although its complexity make it challenging as well as fascinating. The interest in field of quantum technology, quantum physics and nanotechnology motivates for this investigation.

4. Hypothesis

Hydrogenic impurity states creates localized states in low dimensional systems like Quantum dots with different geometries and quantum wires of varying geometrical structures which leads to the various phenomena like quantum confinement effect, carrier localization etc. due to which change in energy spectrum can be observed and different physical properties like carrier mobility, optical absorption, magnetic ordering etc. could be enhanced of such type of low dimensional nanomaterials.

5. Research design and methodology

This research will employ both theoretical and computational approaches. In this research on impurity states in nanostructures, quantum mechanical approximation methods play a crucial role in analyzing and predicting impurity-host interactions. These methods help to simplify complex quantum systems that cannot be solved exactly. Below is a brief introduction to the key quantum mechanical approximation techniques may be used in this study, along with their relevant equations and formulae.

5.1 Perturbation Theory

Perturbation theory is used to approximate the behavior of quantum systems [12] where the Hamiltonian $\hat{H}$ can be expressed as a sum of an exactly solvable part $\hat{H}_0$ and a small perturbation $\hat{V}$:

$$\hat{\mathbf{H}} = \hat{\mathbf{H}}_{\mathbf{0}} + \hat{\boldsymbol{V}}$$

This method is particularly useful for understanding how impurities (considered as small perturbations) modify the energy states of the system. The energy correction for the n-th state in first-order perturbation theory [12,13] is given by:

$$\boldsymbol{E_n^{(1)}} = \langle \boldsymbol{\psi_n^0} | \hat{\boldsymbol{V}} | \boldsymbol{\psi_n^0} \rangle$$

where $\boldsymbol{\psi_n^0}$ is the unperturbed wave function.

5.2 Variational Method

The variational method is used to study the approximated ground state energy of a quantum system. It relies on the variational principle. This principle states that the expectation value of the Hamiltonian $\hat{H}$ with any trial wave function Ψ_{trial} provides an upper bound to the true ground state energy E_0 [14,15]:

$$\boldsymbol{E_{trial}} = \frac{\langle \boldsymbol{\Psi_{trial}} | \hat{\mathbf{H}} | \boldsymbol{\psi_{trial}} \rangle}{\langle \boldsymbol{\Psi_{trial}} | \boldsymbol{\Psi_{trial}} \rangle} \geq \boldsymbol{E_0}$$

This method is particularly useful for studying impurity states, where the exact wavefunction is unknown, but a reasonable approximation can be made.

5.3 WKB Approximation

The Wentzel-Kramers-Brillouin (WKB) approximation is useful for semi-classical analysis of quantum systems. It is particularly used for tunneling phenomena. The wavefunction in regions of varying potential is approximated as

$$\Psi(x) \approx \frac{C}{\sqrt{k(x)}} e^{\pm i \int k(x)dx} \quad \text{Where, } k(x) = \frac{\sqrt{2m(E-V(x))}}{\hbar}$$

This method is useful for studying impurity states in systems with potential barriers, such as quantum wells, where tunneling and bound states play a key role[16].

5.4 Effective Mass Approximation (EMA)

Effective mass approximation is a simpler approach for the treatment of elctron in semiconductors and nanostructures. An effective mass is used for charge carriers near conduction or valence band edge to replace the complicated band structure in this method. The Hamiltonian in the EMA is given by:

$$\hat{H} = -\frac{\hbar^2}{2m^*}\nabla^2 + V(r)$$

Where m^* is the effective mass of the electron and V(r) is the potential energy, which may include contributions from impurities [17,18]. This approximation is useful for low-dimensional systems, where confinement effects dominate.

5.5 Tight-Binding Approximation

The tight-binding method is useful for systems where electrons are tightly bound to atoms, such as in low-dimensional materials like 2D materials and nanowires. In this approximation,

the wavefunction is written as a linear combination of atomic orbitals, and the Hamiltonian is simplified to describe hopping between neighboring atoms. The tight-binding Hamiltonian is [19,20]:

$$\widehat{\boldsymbol{H}} = \sum_{\boldsymbol{i}} \in_{\boldsymbol{i}} \boldsymbol{C}_{\boldsymbol{i}}^{\dagger} \boldsymbol{C}_{\boldsymbol{i}} + \sum_{\langle \boldsymbol{i},\boldsymbol{j} \rangle} \boldsymbol{t}_{\boldsymbol{ij}} \boldsymbol{C}_{\boldsymbol{i}}^{\dagger} \boldsymbol{C}_{\boldsymbol{j}}$$

where $\in_i$ is the on-site energy, t_{ij} is the hopping term, $C_i^{\dagger}$ and C_j are creation and annihilation operators. This method is widely used for studying impurity effects in crystalline and low-dimensional systems.

These theoretical methods will be tested to solve the problem. Any one method which will most suit to our problem will be used to investigate our proposed research work.

The analytical/numerical solutions so obtained would be computed writing codes in PYTHON/MATLAB/SCILAB. Attempts will be made to analyze the results and corroborate the same with available data from other sources.

6. Significance of the Study

The study of impurity states in nanostructures holds profound significance for both fundamental science and practical applications in modern technology.

6.1 Relevance to present day problem

In modern era as the dimensions of materials shrink to the nanoscale, impurities whether introduced deliberately (through doping) or unintentionally (as defects) exert a much stronger influence on the material's physical properties compared to their bulk counterparts [21]. Comprehending these effects is essential for the design and enhancement of nanodevices across a range of advanced technological fields.

6.2 Need of the society

The study of hydrogenic impurity states in low dimensional nanomaterials like quantum dot and quantum wires can help in design of high performance transistors, electronic devices, improved optoelectronic devices etc. As these devices are ecofriendly, low costing and renewable source of energy these qualities make them a great technological tool for sustainable environmental and scientifically developed society.

6.3 Contribution to the existing knowledge

This study will help to devlop deeper understanding of effect of hydrogenic impurity states in nanoscale materials with various geometrical structures and will help to solve the new problems and complexity arising at this nanoscale level. This study also gives a chance to explore a bit more with quantum physics and solid state physics.

7. Future Work

Our proposed research work may be useful for various fields like insights into fundamental physics of nano systems, advancement of semiconductor technology, development of quantum computing and spintronics [22-25].

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